No. T-15/66

Technical Memorandum

NOTES ON QUASI-WUNDY CODE

James P. Coughlin

Warhead and Terminal Ballistics Laboratory

U. S. Naval Weapons Laboratory

Dahlgren, Virginia

UNCLASSIFIED
Security Classification

DOCUMENT CONTROL DATA - R & D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY *(Corporate author)* Naval Weapons Laboratory Dahlgren, Virginia 22448	2a. REPORT SECURITY CLASSIFICATION UNCLASSIFIED 2b. GROUP

3. REPORT TITLE

NOTES ON QUASI-WUNDY CODE

4. DESCRIPTIVE NOTES *(Type of report and inclusive dates)*

5. AUTHOR(S) *(First name, middle initial, last name)*

James P. Coughlin

6. REPORT DATE	7a. TOTAL NO. OF PAGES	7b. NO. OF REFS
December 1966		

8a. CONTRACT OR GRANT NO.	9a. ORIGINATOR'S REPORT NUMBER(S)
b. PROJECT NO.	TM-T-15/66
c.	9b. OTHER REPORT NO(S) *(Any other numbers that may be assigned this report)*
d.	

10. DISTRIBUTION STATEMENT

Approved for public release; distribution unlimited.

11. SUPPLEMENTARY NOTES	12. SPONSORING MILITARY ACTIVITY

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DD FORM 1 NOV 65 1473 (PAGE 1)

S/N 0101-807-6801

UNCLASSIFIED
Security Classification

14 KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT

DD FORM 1 NOV 65 1473 (BACK)
(PAGE 2)

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Approved by:

R. I. Rossbacher

R. I. ROSSBACHER
Director, Warhead and Terminal
Ballistics Laboratory

While the contents of this memorandum are considered to be correct, they are subject to modification upon further study.

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ABSTRACT

A derivation is presented of the basic equations of the Quasi-Wundy Code; this code is widely used for computer calculations relating to explosive systems. The paper begins with the basic notions and attempts to clear up the confusion concerning Lagrangian and Eulerian equations which is all too common in the literature. A brief derivation of the fundamental equations of continuum mechanics follows and these equations are then differenced to give the equations of the code in the form actually employed in the code. The computational procedure is then discussed and two questions which often arise with respect to the working of the code are answered. It is hoped that this paper will provide a background for answering other questions as they arise.

FOREWORD

The wide use of the Quasi Wundy Code for various calculations relating to explosive systems has shown the need for an adequate summary of the basic equations and computational schemes of the code together with the derivations behind them. To the best of the author's knowledge, such information has not been documented and is not readily available from any source, although it is necessary in order to answer some of the questions which arise with respect to use of the code. Answers to two such questions have been included in the body of the report and it is hoped, that sufficient insight into the code is generated to prepare the reader to answer any other questions which may arise.

This paper should serve, further, both to introduce the reader to the code as well as to make known its full possibilities so that individual investigators can adapt it to their own special problems. In accordance with this goal, the paper proceeds from basic notions of fluid mechanics to the Fortran statements of the code. Some material of a rather basic nature has been included, but it is felt that this is worthwhile since it leaves the paper more nearly self contained thus ensuring uniformity of notation and circumventing the difficulty of obtaining good reference material.

ACKNOWLEDGEMENT

The author acknowledges the contributions of the personnel of NOL, White Oak from whom the code was obtained and especially that of Mr. Dante Piacesi who was very cooperative in answering the many questions that arose in the course of this paper.

Thanks are also due to A. Hankinson for his cooperation and for the use of his report (which is to be published at a later date).

I. BASIC NOTIONS AND COORDINATE SYSTEMS

The Quasi Wundy Code is a one dimensional computer code designed to calculate various quantities of interest in an explosive system. It is assumed that all materials involved obey certain basic equations of fluid mechanics which express the basic conservation laws: energy, momentum and mass.

In order to obtain these equations, it is necessary to make a few preliminary remarks. The first concerns the description of the system which is reacting. There are two possible ways of specifying physical quantities such as pressure and density. The first is simply to set up a coordinate system and locate a point (x,y,z) in that coordinate system. Then the pressure (for example) is defined as some function of the coordinates of the point, (x,y,z) and the time. This is the Eulerian approach.

A second alternative is to identify each particle of fluid, not by its present location relative to a set of fixed coordinates, but by the location at time $t = 0$. This identifies each particle of the fluid in terms of its original location. This is the Lagrangian approach.

In both cases, a set of fixed axes are chosen and the motion is described relative to these fixed axes. The difference lies in the choice of independent variables. Euler chooses the location in space and time and seeks to determine pressure, density, etc. at that point. Lagrange chooses the initial coordinates of the "particle" of fluid and seeks to determine its present location, the pressure, density and so on. It is to be emphasized that, mathematically, the difference between these two approaches is a difference in viewpoint.

The solution to the Lagrange equations include $x = f(a,b,c,t)$ as the x coordinate of the present position of the particle. This is the Euler coordinate, x. Conversely, the solutions to the Eulerian equations will include a function which will describe the past and future locations of the particle now at the point (x,y,z). Constants of integration will occur which depend upon the position of the particle at $t = 0$. These coordinates are the Lagrange coordinates.

The Lagrange approach is better suited than the Euler for describing the motion of mixtures of fluids with different densities and equations of state, since it is only necessary to assign these properties to the initial state of the fluid; during

the subsequent motion it is quite easy to determine which fluid is described by some calculated value of pressure for example, since the fluid is still labelled with its original coordinates in the Lagrangian scheme.

This point is worth developing in detail since the equations of the code are developed in Lagrangian form while the ordinary approach to fluid mechanics is by the Euler equations. Accordingly we give an example to illustrate this point.

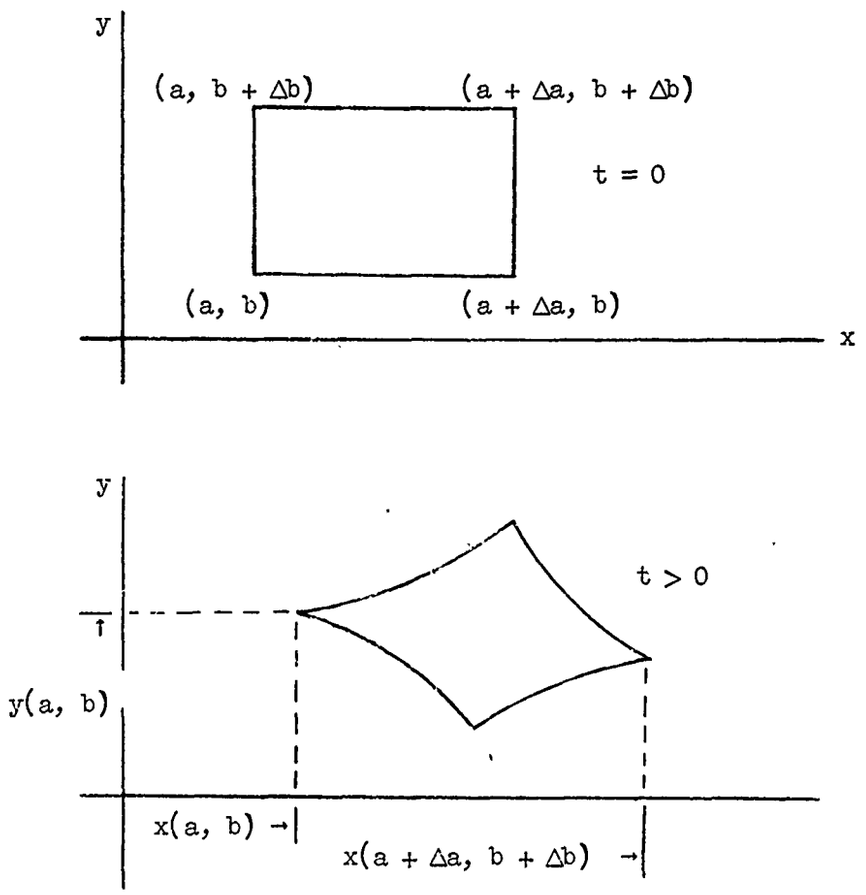


FIGURE 1

In Figure 1, x and y are the Eulerian coordinates and a and b are the Lagrangian coordinates. In the Lagrangian scheme, the particle is characterized by the coordinates a, b and retains these labels for its entire motion. Its location at any time is given by $x = f(a,b,t)$ and $y = g(a,b,t)$. Any physical quantity such as density is determined as a function of a, b, and t: $\rho = \rho(a,b,t)$. This is the present density of the particle which was originally at the point (a,b). If Euler's equations are solved, the solution will include a density equation $\rho = \rho'(x,y,t)$. This is the density of the fluid now at the point (x,y). If (x,y) is the present location of the particle originally at (a,b), we can substitute $x = f(a,b,t)$, $y = g(a,b,t)$ to get

$$\rho = \rho' \left(f(a,b,t),\ g(a,b,t)\ ,\ t\right)$$

The function so obtained is the same as the function obtained from the Lagrange approach.

This point is developed in some detail because of a certain amount of confusion in the literature concerning Lagrangian coordinates. Many statements are given which, though literally accurate, convey a misleading impression. One example is the statement that the Lagrangian reference frame is not inertial. This statement is literally true, since the particles do not change their initial coordinates with time, regardless of the pressures acting. In that sense the coordinate system is not only fixed in the fluid but also distorting as well as moving, with the fluid and hence the Lagrangian mesh of Figure 1b is not inertial. But the reader is cautioned against the error of thinking that the frame of reference for the motion is moving. The frame of reference is the coordinate system with respect to which x and y are measured. These are the Eulerian coordinates and refer to a coordinate system fixed in space, (the fixed axes in Figure 1b).

While the scheme of using the initial coordinates for Lagrangian variables is the simplest and most straightforward approach, it is clear that any function of the initial variables will do equally well. One such function that is used in the scale is the one we will describe next.

Consider the equation

$$M = \int_{x(0,t)}^{x(M,t)} \rho(\xi,t)d\xi$$

where ρ is the fluid density and x, the coordinate of a point in the fluid, is defined as a function of M by the integral. If we take a partial derivative with respect to M on both sides we obtan:

$$1 = \rho(x(M,t),t)\ \frac{\partial x}{\partial M}$$

We consider analogous definitions for the cases of a sphere or an infinitely long cylinder - each of which is a one dimensional problem.

For the cylinder,

$$M = 2\pi \int_{0}^{R(M,t)} \rho(\xi,t)\xi d\xi$$

and

$$1 = 2\pi\ \rho(R(M,t),t)\ R(M,t)\ \frac{\partial R}{\partial M}$$

For the sphere, we have

$$M = 4\pi \int_{0}^{R(M,t)} \rho(\xi,t)\xi^2 d\xi$$

$$1 = 4\pi\ \rho(R(M,t),t)\ [R(M,t)]^2\ \frac{\partial R}{\partial M}$$

where R is the appropriate Eulerian radius.

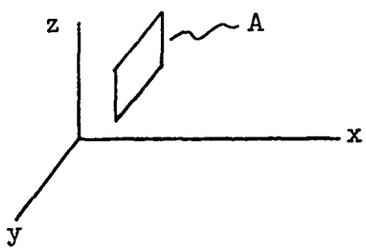
We now introduce a quantity designated by A which represents a surface area. For slab symmetry, we choose an area of unit height and unit width ($\Delta y = 1$, $\Delta z = 1$) and obtain $A(M,t) = 1$.

For a cylinder, we choose unit height Δz and angle 2π to obtain a surface area: $A = 2\pi R(M,t)$ and for a sphere we choose a solid angle of 4π to obtain:

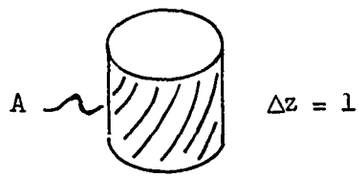
$$A = 4\pi[R(M,t)]^2$$

The diagrams are as follows:

Slab:



Cylinder:



Sphere:

It follows from the law of conservation of mass that the mass contained inside a volume bounded by the same fluid particles is constant in time and depends, therefore, only on the original volume and the coordinates of that volume. Hence the quantity M may be chosen as a Lagrangian coordinate, and the Eulerian coordinate R (or x, in the plane case) is related to it by the differential equation

$$\frac{\partial R}{\partial M} = \frac{1}{\rho(M,t)\ A(M,t)}$$

where $A(M,t) = 1$ for a slab, $A(M,b) = 2\pi\ R(M,t)$ for a cylinder and $4\pi\ R^2$ for a sphere.

With this much noted, we turn our attention to the equations to be solved.

II. EQUATIONS OF THE WUNDY CODE*

We begin our discussion of the Wundy equations with some remarks concerning time derivatives. In order to facilitate our discussion we set $x_1 = x$ $x_2 = y$ and $x_3 = z$ and write x_i as a general term to represent x_1, x_2 or x_3. Similarly, we use a_i to represent a_1, a_2, or a_3 (ie: a, b or c).

Now consider a particle located at the point (x_1, x_2, x_3). In the Lagrangian formulation x_i is a dependent variable and depends on a_i as well as t. But the a_i, which are <u>initial</u> coordinates (or functions thereof), do <u>not</u> depend on time. Hence we write $\dot{x}_i = \frac{\partial x_i}{\partial t}$ and $\dot{x}_i$ is the velocity of the fluid particle at the time t. Similarly, the acceleration is:

$$\ddot{x}_i = \frac{\partial^2 x_i}{\partial t^2}$$

In the Eulerian formulation, the x_i are the independent spatial coordinates but depend on the time. The velocity and acceleration are now given by

$$\dot{x}_i = \frac{dx_i}{dt} \text{ and } \ddot{x}_i = \frac{d^2 x_i}{dt^2}$$

*The reader already familiar with fluid mechanics may easily skip this section.

the difference between the two forms being the same as the difference between partial and total derivatives in ordinary calculus.

As a further illustration, consider the rate at which the density of a given fluid particle changes with time. In the Lagrangian formulation this is simply $\partial\rho/dt$. In the Eulerian formulation this is[1]

$$\frac{d\rho}{dt} = \frac{\partial\rho}{\partial b} + \Sigma_{i=1}^{3} \frac{\partial\rho}{\partial x_i} \frac{dx_i}{dt}$$

or, upon replacing dx_i/dt by the Eulerian velocities:

$$\frac{d\rho}{dt} = \frac{\partial\rho}{\partial t} + \Sigma_{1}^{3} V_i \frac{\partial\rho}{\partial x_i}$$

or in vector form: $\frac{d\rho}{dt} = \frac{\partial\rho}{\partial t} + V \cdot \nabla\rho$

The quantities whose time derivatives we will be seeking are usually integrals and it will be necessary to determine the time derivative of the Jacobian determinant before we can handle them. We suppose the Eulerian coordinates to be related to the Lagrangian coordinates by a set of equations: $x_1 = x_1 (a_1, a_2, a_3, t)$ and the Jacobian determinant of these equations is:

$$J = |T_{ij}|$$

where $T_{ij} = \cdot (\partial x_i/\partial a_j)$ and

$|T_{ij}|$ represents the determinant formed from the elements, T_{ij}.

[1]Note that the x,y,z co-ordinates of a particle are <u>themselves</u> functions of time, hence the total derivative.

To find the derivative of J, we write:

$$\frac{dJ}{dt} = \Sigma_{r,s=1}^{3} \frac{\partial J}{\partial T_{rs}} \frac{dT_{rs}}{dt}$$

The partial derivative of the Jacobian with respect to the element T_{rs} is a rather complex operation and will be set forth in Appendix A for the reader familiar with tensor analysis.

We note the result:

$$\frac{\partial J}{\partial T_{rs}} = \left\{T_{rs}\right\}^{-1} J$$

where the symbol in braces denotes the rs term of the inverse of the matrix formed from the elements T_{rs}. This inverse is simply the matrix $\frac{\partial a_s}{\partial x_r}$. Hence for our time derivative we have:

$$\frac{dJ}{dt} = J \Sigma_{r,s=1}^{3} \frac{\partial a_s}{\partial x_r} \frac{d}{dt} T_{rs}$$

$$= \Sigma_{r,s=1}^{3} J \frac{\partial a_s}{\partial x_r} \frac{d}{dt} \frac{\partial x_r}{\partial a_s}$$

$$= \Sigma_{r,s=1}^{3} J \frac{\partial a_s}{\partial x_r} \frac{\partial}{\partial a_s} \frac{dx_r}{dt}$$

$$= \Sigma_{r,s=1}^{3} J \frac{\partial a_s}{\partial x_r} \frac{\partial}{\partial a_s} u_r$$

$$= J \Sigma_{r=1}^{3} \frac{\partial u_r}{\partial x_r}$$

$$= J \nabla \cdot u$$

With this derivative out of the way, we may turn our attention to the evaluation of time derivatives of integrals. To this end, let ϕ represent any physical quantity characterizing a set of fluid particles. We wish to integrate ϕ over all such particles:

$$I = \iiint_C \phi\,(x,t)\,dv$$

C, being the region comprised of such particles. As the fluid moves, the equation of the boundary changes in time as does ϕ itself. But the Eulerian coordinates of the boundary are functions of the Lagrangian coordinates, a_i, and we can express the integral as an integral over the <u>initial</u> volume of fluid.

$$I = \iiint_{C_o} \phi\,(x(a),t)\,JdV$$

where C_o is the boundary at time zero and J is the Jacobian of the transformation from the a_i to the x_i coordinates.*

Quite obviously, J depends on time, but the bounding surface no longer does since it is evaluated at t = 0.

$$\frac{dI}{dt} = \frac{d}{dt}\iiint_{C_o} \phi\,J\,dV$$

*The reader unfamiliar with Jacobians is referred to Taylor: Advanced Calculus, pages 428-431.

Now since the limits of integration are constants, we can differentiate under the integral sign (assuming ϕ and J are sufficiently smooth) to obtain

$$\frac{dI}{dt} = \iiint_{C_o} \left(\frac{\partial \phi}{\partial t} J + \frac{\partial J}{\partial t} \phi \right) dV$$

$$= \iiint_{C_o} \left(\frac{\partial \phi}{\partial t} J + \phi J \nabla \cdot u \right) dV$$

$$= \iiint_{C_o} \left(\frac{\partial \phi}{\partial t} + \phi \nabla \cdot u \right) J dV$$

$$= \iiint_{C} \left(\frac{\partial \phi}{\partial t} + \phi \nabla \cdot u \right) dv$$

(upon inverting the transformation).

This provides us with all the background material for the conservation laws.

Conservation of mass:

$$\frac{d}{dt} \iiint_{C} \rho \, dv = 0$$

$$\iiint \left(\frac{\partial \rho}{\partial t} + \rho \nabla \cdot u \right) dv = 0$$

and, since this is true for any arbitrary volume, the integrand must be zero.

$$\frac{\partial \rho}{\partial t} + \rho \ \nabla \cdot u = 0$$

Conservation of momentum:

$$\frac{d}{dt}\iiint_c \rho \ u_k \ dv = \Sigma \ F_k$$

where F_k is the k component of the force acting, and the sum is over all forces.

$$\iiint_c \left(\frac{\partial \ \rho u_k}{\partial t} + \rho u_k \ \nabla \cdot u \right) \ dv = \Sigma F_k$$

$$\iiint_c \left[\rho \frac{\partial u_k}{\partial t} + u_k \left(\frac{\partial \rho}{\partial t} + \rho \ \nabla \cdot u \right) \right] dv = \Sigma \ F_k$$

or employing the mass conservation equations:

$$\iiint_c \rho \ \frac{\partial u_k}{\partial t} \ dv = \Sigma \ F_k$$

The forces acting divide into two kinds. The first kind is made up of volume forces such as weight and electromagnetic forces and the second kind is made up of forces acting on the volume at the surface. The hydrodynamic approximation consists in neglecting all forces except those arising from pressure.

Since the pressures are on the order of megabars, there is no problem whatever in dropping all electromagnetic forces and weight forces. In neglecting all viscous forces and rigidity forces in the metals, the program is perhaps open to criticism,

but, nonetheless, the approximation is not as bad as may be anticipated (Reference 1). With this approximation, we write:

$$\iiint_{C} \rho \frac{\partial u_k}{\partial t} \, dv = \iint_{\text{Surface}} - p n_k \, ds$$

where n_k is the k component of the normal vector. The assumption of the hydrodynamic approximation has the effect of reducing the stress tensor of continuum mechanics to a diagonal tensor with the elements of the main diagonal all equal to - p, (ie: $\tau_{ij} = - p \, \delta_{ij}$ in tensor form).

Applying the divergence theorem to the integral at hand, we have:

$$\iiint_{C} \rho \frac{\partial u_k}{\partial t} \, dv = \iiint_{C} - \frac{\partial p}{\partial x_k} \, dv$$

or

$$\iiint_{C} \left(\rho \frac{\partial u_k}{\partial t} + \frac{\partial p}{\partial x_k} \right) dv = 0$$

and finally, since this is true of any volume, we write:

$$\rho \frac{\partial u_k}{\partial t} + \frac{\partial p}{\partial x_k} = 0$$

which is the form of the momentum equation we wish.

The energy equation is also easily derived. We let U be the internal energy per unit mass and let h be a vector representing the heat current out of the surface. (The heat current is defined as that vector which makes the integral

$$\iint_{\text{Surf}} h \cdot \hat{n} \, ds$$

equal to the heat that is transported out of the volume through the surface.) Further, suppose that heat is being generated inside the surface at a rate λ per unit mass. Then applying the first Law of Thermodynamics, the rate at which the energy in the volume changes is equal to the work done on the body by the pressure forces plus the heat generated inside the body (λ, as defined above) minus the heat lost through the surface (heat current, mentioned earlier). In equation form, this statement reads:

$$\frac{d}{dt}\iiint_C \rho\left(U + \frac{1}{2}u^2\right) dv = -\iint_S p\,(n \cdot u)dA - \iint_S h \cdot \hat{n}\, ds$$

$$+\iiint_C \rho\,\lambda\, dv$$

The derivative on the left we evaluate as before:

$$\iiint_C \left[\dot{\rho}\left(U + \frac{1}{2}u^2\right) + \rho\left(\dot{U} + u\dot{u}\right) + \nabla \cdot u\,\rho\left(U + \frac{1}{2}u^2\right)\right] dv$$

$$= \iiint_C \left[\rho\left(\dot{U} + u\dot{u}\right) + \left(U + \frac{1}{2}u^2\right)\left(\dot{\rho} + \rho\,\nabla \cdot u\right)\right] dv$$

$$= \iiint_C \rho\left(\dot{U} + u\dot{u}\right) dv$$

where the mass conservation law has been applied.

Now we have:

$$\iiint_{Vol} \rho\left(\dot{U} + u\dot{u}\right)dv = -\iiint_C \nabla \cdot (pu)\, dv - \iiint_C \nabla \cdot h\, dv$$

$$+\iiint_C \rho\,\lambda\, dv$$

$$\iiint \left[\rho \left(\dot{U} - \lambda \right) + \rho u \dot{u} + \nabla \cdot pu + \nabla \cdot h \right] dv = 0$$

$$\iiint \left[\rho \left(\dot{U} - \lambda \right) + u \cdot \left[\rho \dot{u} + \nabla p \right] + p \, \nabla \cdot u + \nabla \cdot h \right] dv = 0$$

$$\iiint_c \left[\rho \left(\dot{U} - \lambda \right) + p \, \nabla \cdot u + \nabla \cdot h \right] dv = 0$$

where the momentum conservation law has been employed. Since the integral vanishes for every volume, it follows that:

$$\rho \left(\dot{U} - \lambda \right) + p \, \nabla \cdot u + \nabla \cdot h = 0$$

For the Wundy code, the heat conducted away is assumed negligible and $h \simeq 0$. The source of heat is assumed to be viscosity and is incorporated into the pressure term by the introduction of an artificial viscosity term, q (Reference 2). This term is the very core of the solution. By manipulating it properly, we arrive at a continuous solution for the variables. The shock discontinuity which appears is smoothed out over a few zones and it becomes possible to find difference equations whose solutions will approximate the revised problem. We will discuss q at a later point in the paper but, for the present, we merely note that $- \rho \lambda = q \, \nabla \cdot u$. Solving for $\dot{U}$, we obtain $\rho \dot{U} = - (p+q) \, \nabla \cdot u$. Using the mass conservation equation, we can eliminate $\nabla \cdot u$ to get:

$$\nabla \cdot u = \frac{1}{\rho} \frac{\partial \rho}{\partial t}$$

$$\dot{U} = (p+q) \frac{1}{\rho^2} \frac{\partial \rho}{\partial t}$$

If we introduce the specific volume $V' = 1/\rho$, we obtain:

$$\dot{U} = - (p+q) \frac{\partial V'}{\partial t}$$

Summarizing, our equations read:

mass:

$$\frac{\partial \rho}{\partial t} + \rho \nabla \cdot u = 0$$

momentum:

$$\rho \frac{\partial u_k}{\partial t} = - \frac{\partial p}{\partial x_k}$$

energy:

$$\frac{\partial U}{\partial t} = - (p+q) \frac{\partial V'}{\partial t}$$

The first of these equations is open to objection, since there is little point in obtaining differential equations in the density. An alternative approach is to introduce the mass variable introduced at the end of the first section. Recall that

$$M = \int_{x(o,1)}^{x(M,t)} \rho(\xi,t) A(\xi) \, d\xi$$

and

$$\frac{\partial x}{\partial M} = \frac{1}{\rho A} .$$

With this variable, the conservation of mass is automatic since each particle is permanently identified by the mass contained between the initial particle and the particle in question.

The other conservation laws, take the form:

Momentum: $\rho \frac{\partial u}{\partial t} = - \frac{\partial p}{\partial x} \frac{\partial x}{\partial M} \rho A$ or $\frac{\partial u}{\partial t} = - A \frac{\partial p}{\partial M}$

Energy: $\frac{\partial U}{\partial t} = - (p+q) \frac{\partial V'}{\partial t}$ (as before)

To obtain the equations of the code, we must multiply this last equation by ρ_o and set $\rho_o U = E$ and $\rho_o V' = V$. Since ρ_o, the initial density, is constant we have:

$$\frac{\partial E}{\partial t} = - (p+q) \frac{\partial V}{\partial t}$$

and the momentum equation is unaltered:

$$\frac{\partial u}{\partial t} = - A \frac{\partial p}{\partial M}$$

To these two equations of motion we add the <u>supplementary equations</u>:

$$V = \rho_o / \rho$$

$$\dot{u} = \partial u / \partial t$$

$$u = \partial r / \partial t$$

<u>Definitions</u>: Area = $\begin{cases} 1 & \text{slab} \\ 2\,R & \text{cylinder} \\ 4\,R^2 & \text{sphere} \end{cases}$

Volume = $\begin{cases} R_o - R_i & \text{slab} \\ \pi(R_o^2 - R_i^2) & \text{cylinder} \\ \frac{4\pi}{3}(R_o^3 - R_i^3) & \text{sphere} \end{cases}$

(The subscripts i and o refer to inner and outer boundaries respectively of the region of interest).

<u>Equation of State</u>: $p = F(E,V)$

The equation of state is a thermodynamic equation relating (in our case) the pressure, internal energy and reduced density. We will discuss various equations of state somewhat later in this report.

III. DIFFERENCED FORM OF THE EQUATIONS

The basic notion behind the use of high speed computers to solve differential equations is the replacement of the derivatives involved by difference quotients which approximate the derivative. Thus to solve the equation:

$$\frac{dy}{dx} = x \qquad y(x_o) = y_o$$

we assign Δx a value and compute Δy from the equation: $\Delta y/\Delta x = x_o$. The variable y is the increased from y_o to $y_o + \Delta y$ and x is increased to $x_o + \Delta x$. The process is then repeated and a column of corresponding x and y values are produced.

Similar observations apply to partial differential equations, except that there are more variables. To this end we number the space variable, in this case the mass, by the number J. The time is represented by the number n. Thus $\frac{\partial \phi}{\partial t}$ is represented by:

$$\left(\phi_J^{N+1} - \phi_J^N \right) \Big/ \Delta t$$

and

$$\partial\phi/\partial M \text{ by: } \left(\phi_{J+1}^N - \phi_J^N \right) \Big/ (M_{J+1} - M_J)$$

To facilitate the writing, we employ $\phi(J,N)$ to represent ϕ_N^J hereafter.

The computation proceeds by calculating all the quantities desired at the time n for each mass cell. The spatial computations are performed first at a fixed time, then the time is advanced and the process repeated.

Fractional indices are introduced in order to "center" the difference scheme. In this fashion, a higher accuracy can be achieved with the same number of zones. The quantity $\phi\ (J + 1/2)$ is a value of ϕ intermediate between $\phi(J)$ and $\phi(J+1)$. To illustrate their use, let us take a differenced form of the equations derived in part 2. We write these equations down and comment on them later.

Conservation of Energy:

$$\frac{\partial E}{\partial t} = -(p+q)\frac{\partial V}{\partial t}$$

$$E(J-1/2, N+1) = E(J-1/2, N) - \frac{1}{2}\left\{\left[p(J-1/2, N) + P(J-1/2, N+1)\right] + q(J+1/2, N+1/2)\right\}\left[V(J-1/2, N+1) - V(J-1/2, N)\right]$$

Momentum:

$$\frac{\partial u}{\partial t} = -A\ \partial p/\partial M$$

$$DUDT = -A(J,N)\ \frac{(p+q)(J+1/2,N) - (p+q)(J-1/2,N)}{M(J+1/2) - M(J-1/2)}$$

where DUDT is the computer name for the acceleration. This expression is equivalent to:

$$DUDT = A(J,N)\ \frac{(p+q)(J-1/2,N) - (p+q)(J+1/2,N)}{1/2\ [M(J+1/2) + M(J-1/2)]}$$

Defining Relations:

$V = \rho_o/\rho$

$$V(J-1/2, N+1) = \rho_o\ Vol(J-1/2, N+1) / m(J-1/2)$$

$u = \frac{\partial x}{\partial t}$

$$x(J, N+1) = x(J, N) + u(J, N+1/2) \cdot \Delta T_{min}$$

$$DUDT = \frac{\partial u}{\partial t}$$

$$u(J, N + 1) = u(J, N) + DUDT \, \Delta T_{min}$$

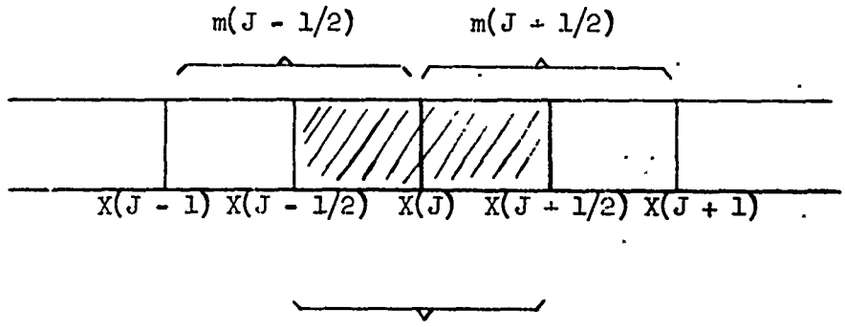
$$\text{Area} = \begin{matrix} 1 \\ 2\pi X \\ 4\pi X^2 \end{matrix} \qquad A(J, N + 1) = \begin{matrix} 1 \\ 2\pi X(J, N + 1) \\ 4\pi X^2(J, N + 1) \end{matrix}$$

$$\text{Vol} = \begin{matrix} (R_o - R_1) \\ \pi(R_o^2 - R_1^2) \\ 4\pi/3(R_o^3 - R_1^3) \end{matrix}$$

$$\text{Vol}\,(J - 1/2, N + 1) = \begin{matrix} X(J, N + 1) - X(J - 1, N + 1) \\ \pi[X^2(J, N + 1) - X^2(J - 1, N + 1)] \\ 4\pi/3\,[X^3(J, N + 1) - X^3(J - 1, N + 1)] \end{matrix}$$

These are the basic equations of Wundy as set forth in section 2. The superscript n refers to the time and the subscript j to the distance. The subscript $j - \frac{1}{2}$ identifies a variable as in the space bounded by the two lines R_j and R_{j-1}.

The quantity $m(J - 1/2)$ is the mass contained in the zone between $X(J)$ and $X(J - 1)$. It is obtained from the previous mass variable M by the relation $m(J - 1/2) = M(J) - M(J - 1)$. The expression $M(J + 1/2) - M(J - 1/2)$ should be taken to mean the difference between two masses. The first mass is that contained between the left hand boundary of the initial particle and the surface corresponding to $X(J + 1/2)$. The second is the mass between the same initial boundary and the surface corresponding to $X(J - 1/2)$. This is best understood by reference to the following diagram:



Since $M(J + 1/2) - M(J - 1/2)$ is the sum of the masses lying between $X(J - 1/2)$ and $X(J)$ on the one hand and between $X(J)$ and $X(J + 1/2)$ on the other. If $X(J - 1/2)$ and $X(J + 1/2)$ divide the regions $X(J - 1) - X(J)$, $X(J) - X(J + 1)$, into two halves with equal masses, then the mass between $X(J - 1/2)$ and $X(J)$ will be half the mass of the entire region $X(J - 1) - X(J)$, that is $1/2\ m(J - 1/2)$. Similarly the other mass involved is $1/2\ m(J + 1/2)$, so that $M(J + 1/2) - M(J - 1/2) = \frac{1}{2}(m(J + 1/2) + m(J - 1/2))$.

With this in mind, it is obvious that the two expressions for DUDT in the difference equations are equivalent.

At this point, the question arises whether the differential equations could be represented by another set of difference equations. The answer to this question is yes. Fromm (Reference 8) considers several schemes of differencing and evaluates them. Unfortunately, Fromm's criterion for evaluation is basically a stability criterion. He considers the best equation to be the one that allows the largest Δt to be used before instability sets in. While this may be a good mathematical criterion, the obvious physical criterion of agreement between calculated and observed values has not yet been fully employed.

As an example of the alternatives available, the following extract from Fromm's work is given:

1) $X(J - 1/2, N + 1) = X(J - 1/2, N) + u(J - 1/2, N)\ \Delta t$

2) $X(J - 1/2, N + 1) = X(J - 1/2, N) + \frac{1}{2}\left[u(J - 1/2, N + 1) + u(J - 1/2, N)\right] \Delta t$

3) $X(J - 1/2, N + 1) = X(J - 1/2, N) + u(J - 1/2, N + 1)\ \Delta t$

Of these equations, Fromm's work indicates that the last is preferable. On physical grounds, however, it seems that some sort of average velocity would yield the best results in the computation of the final position, since this would represent the velocity of the zone at some intermediate time. There is also a tendency to choose the initial value of velocity partly because we ordinarily extrapolate from present knowledge (u(N) and X(N)) to future knowledge X(N + 1). Physically Fromm's choice of the best equation runs counter to the normal choice.

By considering a Taylor expansion of X as a function of time, we will gain some insight into the difference equations. Accordingly, we write:[1] (using superscripts and subscripts throughout for clarity.

$$X^{N+1}_{J-1/2} = X^{N+1/2}_{J-1/2} + \frac{\Delta t}{2}\left(\frac{\partial x}{\partial t}\right)^{N+1/2}_{J-1/2} + \frac{\Delta t^2}{8}\left(\frac{\partial^2 x}{\partial t^2}\right)^{N-1/2}_{J-1/2} + \cdots$$

$$X^{N}_{J-1/2} = X^{N+1/2}_{J-1/2} - \frac{\Delta t}{2}\left(\frac{\partial x}{\partial t}\right)^{N+1/2}_{J-1/2} + \frac{t^2}{8}\left(\frac{\partial^2 x}{\partial t^2}\right)^{N+1/2}_{J-1/2} + \cdots$$

Upon subtracting these, we obtain:

$$X^{N+1/2}_{J-1/2} - X^{N}_{J-1/2} = \Delta t \left(\frac{\partial x}{\partial t}\right)^{N+1/2}_{J-1/2} + O(\Delta t)^3$$ and the most

accurate representation for fixed Δt ought to be:

[1]Note that fundamental time increment Δt is the time from cycle N to cycle N+1. Since we have used cycle N+1/2, the time difference between the 2 cycles is $\Delta t/2$.

$$X^{N+1}_{J-1/2} = X^{N}_{J-1/2} + \Delta t \left(\frac{\partial x}{\partial t}\right)^{N+1/2}_{J-1/2}$$

$$= X^{N}_{J-1/2} + \Delta t \cdot u^{N+1/2}_{J-1/2}$$

But, as Fromm points out, the error introduced by neglecting terms of higher order may actually be lower in the case where u^{N+1} because the neglected terms tend to cancel each other out in one case and not in the other.

Similar differencing schemes may be tried on all the equations, but the scheme used in Wundy is the only one that need concern us here.

Since the difference equations are not the same as the differential equations they represent, but only an approximation to the differential equations, the solutions to the difference equations are not the same as the true solutions but only an approximation. It is reasonable to suppose that the solutions to the difference equations can be made as close as we please to the true solutions by choosing Δt sufficiently small and making $m(J + 1/2)$ sufficiently small. But non-linear differential equations are rather ornery objects and have a way of confounding predictions of this kind. In our case, however, the two solutions can be made arbitrarily close providing only that (1) Δt and $m(J + 1/2)$ are chosen sufficiently small and (2) that the system of difference equations is stable, the theorem (stating that stability of a system of difference equations is necessary and sufficient for convergence of the solution of these equations to the true solution) being due to Peter Lax (References 3 and 6).

The stability of a system of difference equations refers to the amplification of errors introduced into the computing process by various means - round-off errors, inaccurate data and so on. If such errors are amplified and grow in time as the computation proceeds, the difference equations are said to be unstable. If not the equations are stable. Striking examples of numerical instability are given by Richtmeyer (Reference 3) and the following example is taken from the source.

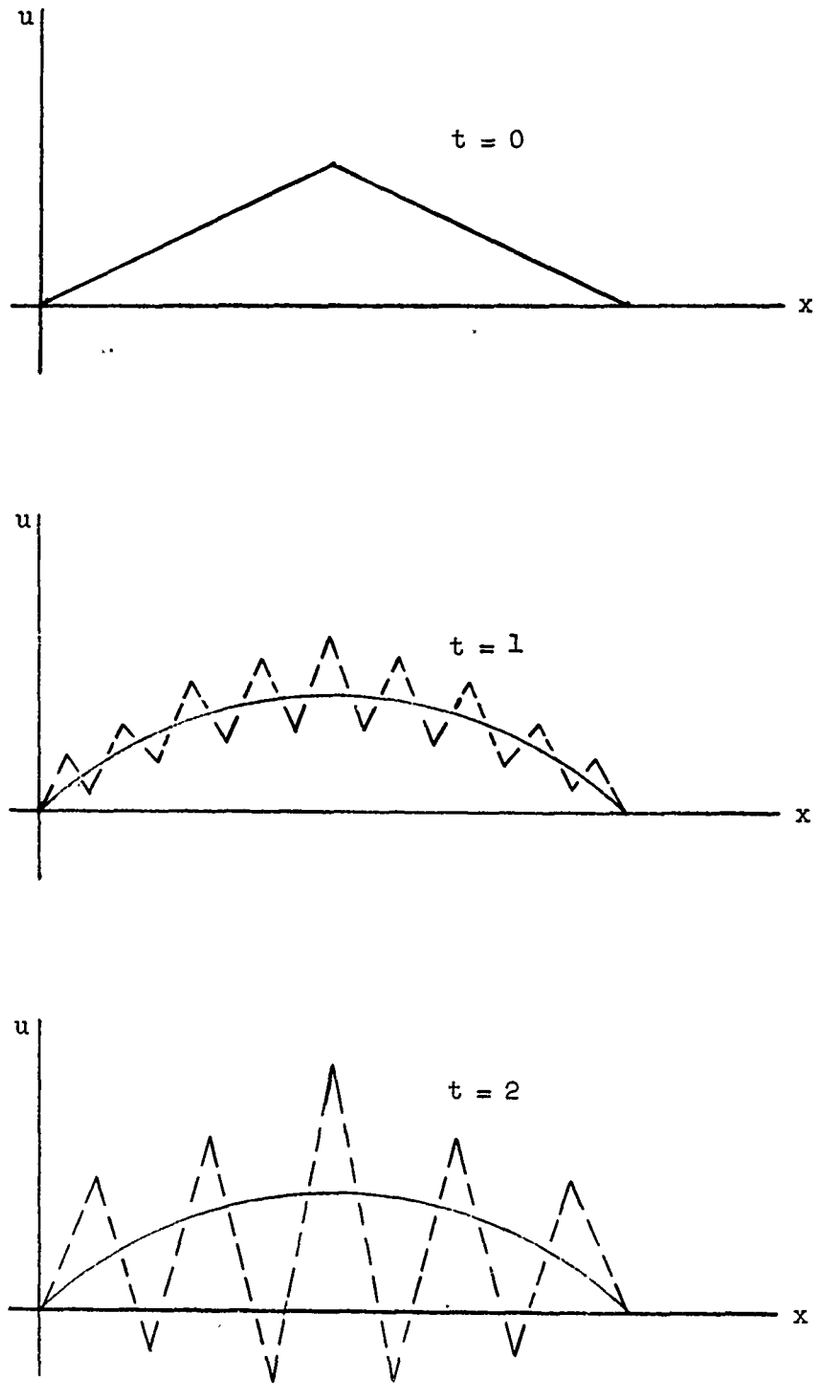


Figure 3

The continuous lines represent the solution to a differential equation and the dashed lines the solution to the difference equations. It is obvious that the two solutions are not approaching one another as t increases.

Instability is avoided by insuring that a certain relation holds between the increments to the distance and time variables. Courant, Friedrichs and Lewy deduced the first stability criterion and Von Neumann and Richtmeyer have applied this criterion to the Wundy code. The criterion is automatically satisfied by the DELTAT subroutine which computes Δt - the change in time from 1 cycle to the next. It is important to note that no stable set of difference equations exists to describe the problem with a shock discontinuity present. This is why the artificial viscosity was introduced.

The functional form of the artificial viscosity is rather arbitrary but the following conditions are imposed:

(1) When the artificial viscosity term is incorporated into the problem, the equations must have continuous solutions.

(2) The distance over which the shock is spread must be everywhere on the order of the thickness of the zones used in the numerical computation, independently of the shock strength (so that the same q will work for all shocks) and independently of the condition of the material into which the shock is moving (so that q is determined solely by the variables which influence the pressure, density, velocity and the other physical quantities involved).

(3) Outside the shock front, the effect of q must be negligible. This is to be taken to mean that the difference between the quantities computed with the use of q and the quantities computed by more exotic schemes will be negligible, which implies that q itself is small.

(4) The Hugoniot equations must hold when all other dimensions are large compared to the shock thickness.

von Neumann and Richtmeyer discovered that, for 1 dimensional flow in a substance which obeyed the γ law expression:

$$q = - \frac{(C\Delta x)^2}{V'} \frac{\partial u}{\partial x} \cdot \left|\frac{\partial u}{\partial x}\right|$$

satisfied all these conditions. A later correction was made setting $q = 0$ for $\frac{\partial u}{\partial x} \geq 0$. For if $\partial u/\partial x$ is non-negative then the front of the zone is moving more rapidly than the rear and the zone is expanding. In this case, no shock is formed or likely to form and consequently the undisturbed equations have a continuous solution and there is no need of the smoothing effect of q. The form of q used in Wundy is:

$$q = - \frac{(C\Delta x)^2}{V'} \left|\frac{\partial u}{\partial x}\right| \frac{\partial u}{\partial x} \qquad \text{if } \frac{\partial u}{\partial x} < 0$$

But $V' = V/\rho_o$ so that

$$q = \frac{(C\Delta x)^2}{V} \rho_o \left(\frac{\partial u}{\partial x} \right)^2$$

$q(J - 1/2, N + 1/2)$

$$= \rho_o (I) \frac{C^2 [u(J, N + 1/2) - u(J - 1, N + 1/2)]^2}{V(J - 1/2, N + 1/2)}$$

$$= C^2 \frac{\rho_o (I) [u(J, N + 1/2) - u(J - 1, N + 1/2)]^2}{\frac{1}{2} [V(J - 1/2, N + 1) + V(J - 1/2, N)}$$

Using the code symbol CQSQX4, we set von Neumann's C^2 = CQSQX4/4 to obtain:

$$q(J - 1/2,\ N + 1/2)$$

$$= \frac{CQSQX4}{4} \frac{\rho_o\ (I)[u(J,\ N + 1/2) - u(J - 1,\ N + 1/2)]^2}{\frac{1}{2}[V(J - 1/2,\ N + 1) + V(J - 1/2,\ N)]}$$

$$= \frac{CQSQX4}{2} \frac{\rho_o\ (I)[u(J,\ N + 1/2) - u(J - 1,\ N + 1/2)]^2}{[V(J - 1/2,\ N + 1) + V(J - 1/2,\ N)]}$$

and CQSQX4 (I) is set equal to 9 for explosives and 16 for metals in the present code.

IV. EQUATIONS OF STATE

The equations of state are normally determined empirically. For explosive gases, the equation used is the ideal gas equation:

$$pV = RT;\ E - E_o = C_vT$$

where E is the internal energy per mole and p,V,T R and C_v all have their usual significance and refer to 1 mole of gas. (Refer to Zemansky: Heat and Thermodynamics, page 120) Recall $C_p - C_v = R$ and $C_p/C_v = \gamma$ and we have:

$$A - A_o = C_v \frac{pV}{R} \quad \frac{C_v}{C_p - C_v}\ pV$$

$$= \frac{1}{\gamma - 1}\ pV$$

Dividing both sides by the atomic weight in grams, on the left we obtain the internal energy per gram (instead of per mole) and on the right, we have the volume of one mole divided by the mass of one mole which is the reciprocal of the density.

$$U - U_o = \frac{1}{\gamma - 1}\ p/\rho$$

Multiply by ρ_o - the initial density and the result is:

$$E - E_c = \rho_o (U - U_o) = \frac{1}{\gamma - 1} p (\rho_o/\rho)$$

or

$$E - E_o = \frac{1}{\gamma - 1} pV$$

where $V = \rho_o/\rho$ as defined earlier.

This equation represents the energy of an ideal gas for $\gamma = 1.4$. For values of γ in the neighborhood of 3*, the equation also represents not only a condensed explosive but also, to a good approximation the high pressure gases released by the detonation process (Reference 7). The energy that is released into the wave is controlled by the burn fraction, F, which is defined as the following ratio:

$$F = \frac{1 - V}{1 - V_{CJ}}$$

where $V = \rho_o/\rho$ and $V_{CJ} = \rho_o/\rho_{CJ}$ the subscript CJ referring to the Chapman-Jouget conditions (Reference 4). If the Chapman-Jouget hypothesis is satisfied, then:

$$(\rho_o/\rho) = \frac{\gamma}{\gamma + 1} = V_{CJ}$$

$$1 - V_{CJ} = 1 - \frac{\gamma}{\gamma + 1} = \frac{1}{\gamma + 1}$$

and

$$F = \frac{1 - V}{1 - V_{CJ}} = (\gamma + 1)(1 - V)$$

which is in the form used in the code. The fraction of the energy released is then F.

*This value of γ need no longer represent the ratio of specific heats in the explosive

In the actual working of the code, the burn fraction is subjected to several tests designed to insure that the computed situation is physically realistic. If $F < .00001$, it is assumed that the difference between F and 0 is due to errors in the calculation. If $F > 1$, it is assumed that the difference in F and 1 is due to the same cause. F is then set equal to 1. If F begins to decrease in time, F is set equal to 1. Finally if F is equal to 1 in every zone, the energy of the explosive is spent and the routine is skipped on the next cycle.

The equation of state and the energy equation are both used in advancing the energy. From the above considerations, we have:

$$\partial p/\partial E = (\gamma - 1)/V$$

or in differenced form:

$$DPDE = (\gamma - 1)/V\ (J - 1/2,\ N + 1)$$

The energy equation of section II is now employed

$$\partial E/\partial t = -\ (p + q)\ \partial V/\partial t$$

to obtain:

$$E(J - 1/2,\ N + 1/2) - E(J - 1/2,\ N)$$
$$= -\ (p + q)(J - 1/2,\ N)\ [V(J - 1/2,\ N + 1)$$
$$- V(J - 1/2,\ N)]$$

But, inside the explosive, this equation is subject to error because energy source terms are not included. Moreover the pressure $p(J - 1/2,\ N)$ is decidedly not the pressure acting over the entire time cycle or even a good approximation to it since the pressure can be expected to increase greatly

when the energy of the detonation is released. For these reasons, an iteration process is used in computing $E(J - 1/2, N + 1)$. First we set

$$EI = E(J - 1/2, N) - (p + q)(J - 1/2, N + 1)\,[V(J - 1/2, N + 1) - V(J - 1/2, N)]$$

$$PI = DPDE \cdot EI \cdot F(J - 1/2, N + 1)$$

These intermediate pressures and energies are then employed in obtaining the resultant pressure and energies as follows:

$$E(J - 1/2, N + 1) = E(J - 1/2, N) - \frac{1}{2}\,[PI - P(J - 1/2, N)] \cdot [V(J - 1/2, N + 1) - V(J - 1/2, N)]$$

$$P(J - 1/2, N + 1) = DPDE \cdot E(J - 1/2, N + 1) \cdot F(J - 1/2, N + 1)$$

The computation, having advanced E and P, returns to the main program.

Of all the inert materials a genuine equation of state is available only for aluminum as of this writing. For other materials, the Hugoniot equation is used. This equation is strictly an equation of process and not of state, the process involved being a shock transition. The Hugoniot is accurate, therefore, only for shock transitions, but very weak shocks are nearly isentropic and, if the drop in pressure from zone to zone is not too great in the relief wave, the Hugoniot will be a good approximation to the adiabat which is the actual curve along which the relief transitions take place.

The Hugoniot (Reference 5) may be obtained from a straightforward empirical curve fitting process or by utilizing the empirical observation that the shock velocity is a linear function of the particle velocity at sufficiently high pressures. The Rankine-Hugoniot equations can then be used to determine the equation of the Hugoniot curve in P - μ coordinates (where μ is the quantity $(\rho/\rho_o - 1)$). A typical calculation of this kind is presented in Appendix B.

The pressure and internal energy are now advanced in a manner similar to that employed for explosives. The intermediate Variables, $p(\mu)$ (in the code language POFMU) and μ (or DMU) are introduced and the empirical relation between them:

$$\text{POFMU} = (C_1 + C_2\ \text{DMU})\ \text{DMU}$$

$$\text{EI} = E(J - 1/2, N) - [P(J - 1/2, N) + q(J - 1/2, N)] \cdot [V(J - 1/2, N + 1) - V(J - 1/2, N)]$$

$$E(J - 1/2, N + 1) = \text{EI} - \frac{1}{2}[\text{POFMU} + C_2\text{EI} - P(J - 1/2, N)] \cdot [V(J - 1/2, N + 1) - V(J - 1/2, N)]$$

$$P(J - 1/2, N + 1) = \text{POFMU} + C_2\ E(J - 1/2, N + 1)$$

If the computed pressure turns out to be less than -3 kilobars, it is set equal to -3 kilobars. Since a tension (negative pressure) of 3 kilobars will cause many metals to fracture, a greater tension cannot appear in the physical explosion. This introduces the negative pressure cutoff.

V. THE PROGRAM

The computation begins by reading off the initial values of the variables from a set of IBM cards. The input variables are:

(1) Equation of state for region J.

(2) Initial density of region J.

(3) The constant CQSQX4 for region J.

(4) The constand γ for region J.

(5) Certain control variables, notably:

(1) MURIN

(2) INV

(3) NALTQ

(4) NSWEEP

(5) K

This list of control variables is by no means exhaustive. These are given as a sample. The control MURIN defines the initial conditions at the innermost boundary. If the geometry is cylindrical or spherical, MURIN = 1. For rectangular (slab) geometry, there are two possibilities, either a rigid wall at the origin (set MURIN = 1) or a free surface MURIN = 0. INV is a control that determines the initial state of the material. If the material is in its normal state, INV = 0. If it is desired to have the material in a compressed state when the program starts, INV is set equal to any number other than zero, (for example INV = 1). Then the ratio of the density in the compressed state to the uncompressed density is read in.

NALTQ is set equal to zero if the von Neumann form of the artificial viscosity q, is desired. If NALTQ $\neq$ 0, then a linear q will be used. This form of q has been used in certain underwater explosion problems at Naval Ordnance Laboratory, White Oak. NSWEEP is a control which introduces a limited calculation procedure. NSWEEP = 0 causes the velocities of three adjacent zones to be tested. If the sum of the absolute values of these three zones is less than 10^{-6}, and the time cycle is less than 2, then it is assumed that the shock has not yet reached those zones and the computation is stopped at the last of these zones.

The last control mentioned, K, determines the geometry of the problem. K = 1 for rectangular, 2 for cylindrical, and 3 for spherical problems.

When all the input values have been read in, all the variables of the calculation (N, J, J + 1/2, etc.) are set equal to their initial values and the patch subroutine (PCH), is called. This subroutine is employed to begin the process. The command PCH(IJ) = TYME alters the value of the

variable in the location IJ to a new value designated by the code word TYME. It has been found most convenient to change the velocity of the first interface to a suitably high value in order to begin the detonation process. With the first zone being compressed, the burn fraction rises and energy is released. This builds up the pressure and the detonation process is underway. Next, the subroutine, GENSUB, is called.

This subroutine sets a series of control variables which locate the various interfaces and any voids that may be present. The program is now ready to go. The limited computation test is applied to determine an upper limit for the calculations. MURIN is then tested to determine the fate of the first zone.

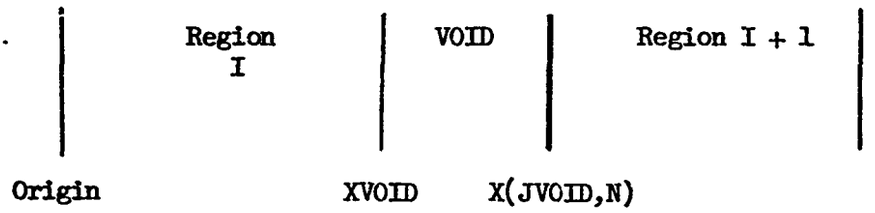
For a rigid wall condition, $u(J, N + 1/2) = u(J, N - 1/2) = TYME$. For a free surface, DUDT is computed and u and x are advanced. The computation now proceeds to advance each zone in accordance with the difference equations cited in section III. The velocity, coordinate, area, reduced density and artificial viscosity are all computed for each zone. At the void closures, the special routines discussed in section VI are employed. When these computations have all been performed, the equation of state is selected and the pressure and internal energy are both advanced. The subroutine DELTAT is called up and a new value of Δt is generated. This value is calculated from stability considerations.

The time is now advanced from t to $t + \Delta t$ and the energy is checked to insure that the total energy does not depart from the initial value of the energy by more than 10%. If it does, the computation is stopped and E WRONG is printed out. (This energy check is optional and is controlled by NCHEKE which is set equal to 1 if this check is desired, and 0 if the check is to be bypassed.) The computer now compares $t + \Delta t$ with the time limit set by the operator. If the run time is larger than $t + \Delta t$, the computation is started all over again using this advanced value of t. If not, the output is summoned and the results of the computation are printed out.

VI. THE VOID SUBROUTINE

The calculations outlined thus far proceed very well in normal situations, but occasionally an extraordinary situation arises and special attention is required. The commonest of these situations occurs when a void is enclosed between two regions.

A new interface must be introduced (XVOID) and appropriate corrections must be made in the equations. The interface on the right where the material begins again is subscripted JVOID and the two collide after a time. The geometry is as follows:



The interface XVOID is advanced as follows:

$$\text{VD DUDT} = \frac{(p+q)(JV-1)}{\frac{1}{2}\,m(J-1/2)} \quad \text{VD AREA}$$

$$\text{UVOID}\,(I, N+1/2) = \text{UVOID}\,(I, N-1/2) + \Delta T\ \text{VDDUDT}$$

$$\text{XVOID}\,(I, N+1) = \text{XVOID}\,(I, N) + \Delta T\ \text{UVOID}\,(I, N+1/2)$$

The first of these equations corresponds to the ordinary differenced form of:

$$\frac{\partial u}{\partial t} = -\ A\ \frac{\partial p}{\partial M}$$

except that, for the void, the pressure in zone $J - 1/2$ is labelled $p(JV - 1)$ and the pressure in zone $J + 1/2$ is set equal to zero (since there is no pressure in a void). Similarly the expression for mass is altered since the zone mass of the void is zero. Thus, only $m(J - 1/2)$ appears.

The right hand boundary is advanced in a similar manner:

$$\text{VJDUDT} = -\frac{(p+q)\ \text{JVOID} \cdot \text{AREA}\,(\text{JVOID}, N)}{\frac{1}{2}\ m(JV)}$$

$$u(JV, N + 1/2) = u(JV, N-1/2) + \Delta T \ VJDUDT$$

$$X(JV, N + 1) = X(JV, N)+\Delta T \ u(JV, N + 1/2)$$

The two X's are now compared to investigate whether the material on the left has overtaken the material on the right or not. If XVOID is still smaller than X(JVOID), then the void is still open and the computation proceeds by advancing X(JV - 1, N + 1), computing a new value of q and returning to the main program. (X(JV - 1, N + 1) is advanced here in order to compute q. It is recomputed later, but it was though best to keep all the void calculations together.)

If XVOID $\geq$ X(JV, N + 1), a void closure has occurred and the program proceeds to compute a new time increment and employs this in subsequent calculations. XVOID is now set equal to zero and the void index JVOID is set equal to -JVOID which serves as a test for void closure. Hereinafter, the subroutine is skipped.

UVOID is advanced from the VDDUDT computation and U(JV, N + 1/2) is also advanced. After X(JV, N + 1/2), the common interface, is advanced, a quantity called UTEMP is introduced. This is the common velocity of the two zones adjacent to the interface X(JV, N + 1) as computed from the usual formula for inelastic collision:

$$UTEMP = \frac{\frac{1}{2} \ m(JV) \ U(JV, N + 1/2) + \frac{1}{2} \ m(JV - 1) \ UVOID}{\frac{1}{2} \ m(JV) + \frac{1}{2} \ m(JV - 1)}$$

X(JV - 1, N + 1) is now advanced just as before and areas, volumes and reduced densities are computed and the computation is returned to the main program.

In the main program, itself, a further correction is made to adjust the energies of these two zones. The mechanical (kinetic) energy lost by the first zone is:

$$\frac{1}{2} \ m(JV - 1) \ (VOID^2 - UTEMP^2)$$

and that gained by the second zone is:

$$\frac{1}{2} \ m(JV) \ (UTEMP^2 - U(JV, N + 1/2)^2)$$

The mechanical energy lost is the difference

$$\frac{1}{4}\Big\{m(JV-1)\,(UVOID^2 - UTEMP^2) + m(JV)\,(U(JV, N+1/2)^2 - UTEMP^2)\Big\}$$

This will appear as thermodynamic energy and a plausible assumption for metals is to assume that this energy is divided equally between the two zones concerned. If we neglect the slight change in density of the metals, we have:

$m(JV)\,(E_o' - E_2)/\rho_2$ = Total change in internal energy of zone JV. ($\frac{\text{energy}}{\text{vol}}$ x mass / density)

$$E_2' - E_2 = (\rho_2/m(JV)\ 1/8\Big\{m(JV-1)\,[UVOID^2 - UTEMP^2] + m(JV)\,[U(JV, N+1/2)^2 - UTEMP^2]\Big\}$$

$$= \frac{1}{4}\left\{\frac{1}{2}\rho_2\,[u(JV, N+1/2)^2 - UTEMP^2] + \frac{1}{2}\rho_2\,\frac{m(JV-1)}{m(JV)}\,[UVOID^2 - UTEMP^2]\right\}$$

And similarly

$$E_1' - E_1 = \frac{\rho_1}{m(JV-1)}\,\frac{1}{8}\Big\{m(JV-1)\,[UVOID^2 - UTEMP^2] + m(JV)[U(JV, N+1/2)^2 - UTEMP^2]\Big\}$$

$$= \frac{1}{4}\left\{\frac{1}{2}\rho_1\,(UVOID^2 - UTEMP^2) + \frac{1}{2}\rho_1\,\frac{m(JV)}{m(JV-1)}\,(U(JV, N+1/2)^2 - UTEMP^2)\right\}$$

For a gas closing on a metal, the low thermal conductivity of the gas is presumed to prevent any appreciable transfer of energy to the metal so that we may neglect ΔE_2 and employ the second equation given above together with the approximation UVOID $\gg$ UTEMP and UVOID $\gg$ U(JV, N + 1/2). Neglecting both these factors and doubling the energy on the right in order to insure that <u>all</u> the mechanical energy lost is converted into thermal energy of the <u>gas</u>, we obtain:

$$E_1' = E_1 + \frac{1}{4}\frac{\rho_1}{m(JV-1)}\,[m(JV-1)\ UVOID^2]$$

$$= E_1 + .5\ (1/2\ \rho_g)\ UVOID^2$$

which is the equation used in Wundy.

When these adjustments have been made, JVOID is set equal to zero and the adjustment is skipped thereafter.

VII. QUESTIONS ON QUASI-WUNDY

There are several questions that arise in the course of working on the Quasi-Wundy code and these will be considered here.

The first of these questions concerns the necessity for mass matching at interfaces between adjacent zones. This question ordinarily arises when a very light metal is placed in contact with a very heavy one and the number of zones required in order to obtain a good notion of the processes occurring in the light metal makes the number of zones in the heavy metal prohibitively expensive if the masses of adjacent zones are matched. As an example, consider a thin aluminum slice - 2.5×10^{-3} cm thick - in contact with a copper plate. The density of aluminum is 2.785 gm/cm^3 and that of copper is 8.93 gm/cm^3. It is estimated that not less than 10 zones are needed in the aluminum in order to get a reliable view of the motions of the shock waves through the aluminum. The thickness of each zone of aluminum is 2.5×10^{-4} cm. Let us consider a unit cross section and the mass of each zone is $2.5\times10^{-4} \times 1 \times 2.785 = 6.9625 \times 10^{-4}$ gm. The copper plate is .635 cm thick and if we require that the mass per zone be 6.9625×10^{-4} gms, we have, for the number of zones:

$$N = \frac{\text{Total mass of Copper}}{\text{mass of zone}} = \frac{1 \times .635 \times 8.93}{6.9625} \times 10^4$$

$$N \simeq 8{,}000$$

The cost of computation for 8,000 zones is rather high. Thus the question naturally arises: Is it necessary to insure that the masses of the zones are equal or nearly so?

Consider the Taylcr expansion of the pressure near a point, m_o, at which the increment Δm is changed. (Normally m_o will be the interface between two regions). According to a well known formula:

$$p(m) = p(m_o) + \frac{\Delta m}{2}\left(\frac{\partial p}{\partial m}\right)_{m_o} + \frac{1}{2!}\left(\frac{\Delta m}{2}\right)^2\left(\frac{\partial^2 p}{\partial m^2}\right)_{m_o} + \frac{1}{3!}\left(\frac{\Delta m}{3}\right)^3\left(\frac{\partial^3 p}{\partial m^3}\right)_{m_o} + \cdots$$

where $m = m_o \pm 1/2\ \Delta m$

Designate $(m_o + \frac{1}{2}\Delta_2 m)$ by $p_{J+\frac{1}{2}}$, $p(m_o - \frac{1}{2}\Delta_1 m)$ by $p_{J-\frac{1}{2}}$ and $(m_o) = p_J$. Then we have:

$$p_{J+\frac{1}{2}} = p_J + \left(\frac{\partial p}{\partial m}\right)_J \frac{\Delta_2 m}{2} + \frac{1}{2!}\left(\frac{\partial^2 p}{\partial m^2}\right)_J \left(\frac{\Delta_2 m}{2}\right)^2 + \frac{1}{3}\left(\frac{\partial^3 p}{\partial m^3}\right)_J \left(\frac{\Delta_2 m}{2}\right)^3 + \cdots$$

$$p_{J+\frac{1}{2}} = p_J - \left(\frac{\partial p}{\partial m}\right)_J \frac{\Delta_1 m}{2} + \frac{1}{2!}\left(\frac{\partial^2 p}{\partial m^2}\right)_J \left(\frac{\Delta_1 m}{2}\right)^2 - \frac{1}{3!}\left(\frac{\partial^3 p}{\partial m^3}\right)_J \left(\frac{\Delta_1 m}{2}\right)^3 + \cdots$$

Subtracting the first expression from the second:

$$p_{J-\frac{1}{2}} - p_{J+\frac{1}{2}} = -\left(\frac{\partial p}{\partial m}\right)_J \left(\frac{\Delta_1 m + \Delta_2 m}{2}\right) + \frac{1}{2!}\left(\frac{\partial^2 p}{\partial m^2}\right)_J \left(\frac{(\Delta_1 m)^2 - (\Delta_2 m)^2}{4}\right)$$

$$- \frac{1}{48}\left(\frac{\partial^3 p}{\partial m^3}\right)_J \left\{(\Delta_1 m)^3 + (\Delta_2 m)^3\right\} + \cdots\cdots\cdots$$

Divide both sides by $\frac{1}{2}(\Delta_1 m + \Delta_2 m)$ and we have:

$$\frac{p_{J-\frac{1}{2}} + p_{J+\frac{1}{2}}}{\frac{1}{2}(\Delta_1 m + \Delta_2 m)} = \left(\frac{\partial p}{\partial m}\right)_J \frac{1}{4}\left(\frac{\partial^2 p}{\partial m^2}\right)_J (\Delta_1 m - \Delta_2 m)$$

$$- \frac{1}{24}\left(\frac{\partial^3 p}{\partial m^3}\right)_J \left[(\Delta_1 m)^2 - (\Delta_1 m)(\Delta_2 m) + (\Delta_2 m)^2\right] + \cdots$$

If $\Delta_1 m \simeq \Delta_2 m$, $\Delta_1 m - \Delta_2 m \simeq 0$ and our equation reads:

$$1) \quad \frac{p_{J-\frac{1}{2}} - p_{J+\frac{1}{2}}}{\frac{1}{2}(\Delta_1 m + \Delta_2 m)} = \left(\frac{\partial p}{\partial m}\right)_J - \frac{1}{24}\left(\frac{\partial^3 p}{\partial m^3}\right)_J O(\Delta m^2)$$

The approximation used in the code is then simply to drop terms of order greater than the second and set

$$2) \quad -\left(\frac{\partial p}{\partial m}\right)_J = \frac{p_{J-\frac{1}{2}} - p_{J+\frac{1}{2}}}{\frac{1}{2}(\Delta_1 m + \Delta_2 m)}$$

and employ this in the equation

$$\frac{\partial u}{\partial t} = -A\frac{\partial p}{\partial m}$$

which advances the velocity and then the X coordinate and hence the density and indirectly the pressure in the next zone.

If the masses are not matched, this equation can be seriously in error.

In an actual run (Quasi-Wundy 84), an attempt was made to match the masses of the zones in the aluminum foil mentioned above and the copper plate. In order to limit computing time an artificial interface was introduced between coarse zoned copper and fine zoned copper. The result showed an attenuation of 150 kilobars in a 400 kilobar shock going from the coarse zoned copper to the fine zoned. In order to explain this spurious effect, consider the neglected terms of equation 1.

$$\sum_{n=2}^{\infty} \frac{1}{2^{n-1}} \frac{1}{n!} \left(\frac{\partial^n p}{\partial m^n}\right)_J \left[- \frac{(\Delta_2 m)^n + (-\Delta_1 m)^n}{\Delta_1 m + \Delta_2 m} \right]$$

The largest of these terms (assuming the series to converge sufficiently rapidly) is the first:

$$E = \frac{1}{2}\frac{1}{2!}\left(\frac{\partial^2 p}{\partial m^2}\right)_J \left[\frac{-(\Delta_2 m)^2 + (\Delta_1 m)^2}{\Delta_1 m + \Delta_2 m}\right]$$

$$E = \frac{1}{4}\left(\frac{\partial^2 p}{\partial m^2}\right)_J (\Delta_1 m - \Delta_2 m)$$

Note carefully that when $\Delta_1 m$ and $\Delta_2 m$ are equal, this expression vanishes and the error is reduced to third order rather than second. It is anticipated that the third order terms are very small. We investigate the lead term. In order to do this, we need an estimate on the derivatives. This is extremely difficult to obtain, but since $(\partial p/\partial m)$ is continuous in the smoothed out shock front (Richtmeyer p203), we will attempt to estimate $\partial p/\partial m$ and $\partial^2 p/\partial m^2$ from the data available although any estimates of higher derivatives probably can not be obtained by the method we will employ. The pressure is initially zero and rises to .4 megabars in the space of four zones - 2 to the left of the interface and 2 to the right. The mass increment to the left of the interface is $\Delta_1 m = .0016$ and to the right is .0001 $(\Delta_2 m)$.

$$\frac{\partial p}{\partial m} \simeq \frac{.4 - 0}{2(.0016) + 2(.0001)} + \frac{.4}{2(.0017)}$$

$$\frac{\partial p}{\partial m} \cong 175$$

To estimate the second derivative, consider that $\partial p/\partial m$ is initially zero and rises to the average value listed above in a space of one zone or so - being smaller than the above value in the first zone and larger in the second so that the average is the quantity listed. In the third zone the derivative begins to decline reaching the average value at the end of the third zone and falling off to zero by the end of the fourth zone.

$$\frac{\partial^2 p}{\partial m^2} \simeq \frac{\partial p/\partial m - 0}{2\Delta_2 m}$$

$$\frac{\partial^2 p}{\partial m^2} \simeq \frac{0 - \partial p/\partial m}{2\ \Delta_1 m}$$

Averaging the absolute values, we get a crude estimate on the maximum value of $\partial^2 p/\partial m^2$:

$$\frac{\partial^2 p}{\partial m^2} \simeq \frac{1}{2}\left[\frac{\partial p/\partial m}{2\,\Delta_1 m} + \frac{\partial p/\partial m}{2\,\Delta_2 m}\right]$$

$$\frac{\partial^2 p}{\partial m^2} \simeq 47 \times 10^4$$

$$E = \frac{1}{2!}\,\frac{1}{2}\,\frac{\partial^2 p}{\partial\, m^2}\quad (\Delta_1 m - \Delta_2 m)$$

$$= \frac{1}{4}(.47 \times 10^4)(.0015)$$

$$\simeq 180$$

which is on the same order as the term $\partial p/\partial m$ which is being calculated. Hence near a shock front, a mass mismatch can introduce a serious error. The calculations listed are by no means sound, they are merely an estimate of possible error. At the present writing, an attempt is being made to eliminate the difficulty, but results are not yet available.

Another question that frequently arises concerns equations of state. As is pointed out in the text, the confusion arises because the Hugoniot is widely used as an equation of state but it is really an equation of process. However, as pointed out in section IV (p26), the Hugoniot is a useful approximation.

VIII. REFERENCES

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APPENDIX A

DERIVATIVE OF THE JACOBIAN DETERMINANT

DERIVATIVE OF THE JACOBIAN DETERMINANT

Let

$$J = \frac{\partial(xyz)}{\partial(abc)} = \left|\frac{\partial x_i}{\partial a_j}\right|$$

$$J = \frac{1}{3!}\,\epsilon_{ijk}\,\epsilon_{emn}\,T_{ie}\,T_{jm}\,T_{km}$$

where $T_{ie} = \frac{\partial x_i}{\partial a_e}$ and the ϵ_{ijk} are the familiar alternating symbols of tensor analysis (see note at end).

$$\frac{\partial J}{\partial T_{rs}} = \frac{1}{3!}\,\epsilon_{ijk}\,\epsilon_{emn}\,\frac{\partial T_{ie}}{\partial T_{rs}}\,T_{jm}\,T_{kn}$$

$$+ \frac{1}{3!}\,\epsilon_{ijk}\,\epsilon_{emn}\,\frac{\partial T_{jm}}{\partial T_{rs}}\,T_{ie}\,T_{kn}$$

$$+ \frac{1}{3!}\,\epsilon_{ijk}\,\epsilon_{emn}\,\frac{\partial T_{kn}}{\partial T_{rs}}\,T_{ie}\,T_{jm}$$

$$= \frac{1}{3!}\,[\epsilon_{ijk}\,\epsilon_{emn}\,\delta_{ir}\,\delta_{es}\,T_{jm}\,T_{kn}$$

$$+ \epsilon_{ijk}\,\epsilon_{emn}\,\delta_{jr}\,\delta_{ms}\,T_{ie}\,T_{kn}$$

$$+ \epsilon_{ijk}\,\epsilon_{emn}\,\delta_{kr}\,\delta_{ns}\,T_{ie}\,T_{jm}]$$

$$= \frac{1}{3!}\,[\epsilon_{rjk}\,\epsilon_{smn}\,T_{jm}\,T_{kn} + \epsilon_{irk}\,\epsilon_{esn}\,T_{ie}\,T_{kn}$$

$$+ \epsilon_{ijr}\,\epsilon_{ems}\,T_{ie}\,T_{jm}]$$

$$= \frac{1}{3!}\,[\epsilon_{rjk}\,\epsilon_{smn}\,T_{jm}\,T_{kn} + \epsilon_{rik}\,\epsilon_{sen}\,T_{ie}\,T_{kn}$$

$$+ \epsilon_{rij}\,\epsilon_{sem}\,T_{ie}\,T_{jm}]$$

Renumbering the dummy indices of summation we obtain:

$$\frac{\partial J}{\partial T_{rs}} = \frac{1}{3!} \left[\epsilon_{r\mu v}\, \epsilon_{sa\beta}\, T_{\mu a}\, T_{v\beta} + \epsilon_{r\mu v}\, \epsilon_{sa\beta}\, T_{\mu a}\, T_{v\beta} + \epsilon_{r\mu v}\, \epsilon_{sa\beta}\, T_{\mu a}\, T_{v\beta}\right]$$

$$\frac{\partial J}{\partial T_{rs}} = \frac{1}{3!} \left[3\, \epsilon_{r\mu v}\, \epsilon_{sa\beta}\, T_{\mu a}\, T_{v\beta}\right]$$

Multiply by T_{ps} and sum on s:

$$T_{ps} \frac{\partial J}{\partial T_{rs}} = \frac{1}{2!}\, \epsilon_{r\mu v}\, \epsilon_{sa\beta}\, T_{\mu a}\, T_{v\beta}\, T_{ps}$$

$$= \frac{1}{2!}\, \epsilon_{r\mu v} \left[\epsilon_{\mu vp}\, J\right]$$

$$= \frac{1}{2!} \left(\epsilon_{\mu vr}\, \epsilon_{\mu vp}\right) J$$

$$= \frac{1}{2!} \left(\delta_{vv}\, \delta_{rp} - \delta_{vp}\, \delta_{vr}\right) J$$

$$= \frac{1}{2!} \left(3\, \delta_{rp} - \delta_{rp}\right) J$$

$$= \frac{2}{2!}\, J\, \delta_{rp}$$

$$= J\, \delta_{rp}$$

So that $T_{ps} \cdot \left[\frac{1}{J}\frac{\partial J}{\partial T_{rs}}\right] = \delta_{pr}$

or $\frac{1}{J}\frac{\partial J}{\partial T_{rs}} = \left[T_{ps}\right]^{-1}$

But $\left[T_{rs}\right]^{-1}$ is obviously $\frac{\partial a_r}{\partial x_s}$ since $\frac{\partial x_s}{\partial a_r}\frac{\partial a_r}{\partial x_p} = \delta_{sp}$.

Hence, as claimed in the body of the report:

$$\frac{\partial J}{\partial T_{rs}} = T_{rs}^{-1}\ J$$

and

$$T_{rs}^{-1} = \frac{\partial a_s}{\partial x_r}$$

NOTE: The summation convention is employed throughout so that $a_{1j}\ b_{jk}$ is summed from J = 1 to 3. The Kronecker δ, δ_{ij}, has the value 1 if i = j and 0 otherwise. Obviously $\delta_{ij}\ a_{jk} = a_{ik}$ for any tensor a. Further $\delta_{jj} = \delta_{11} + \delta_{22} + \delta_{33} = 3$. The alternating symbol ϵ_{ijk} is zero if any 2 indices (i,j,k) are the same. It is one if i j k is an even permutation of 1,2,3 and -1 for an odd permutation.

or

$$[(V'/V'_o) - g]^2 V'^2_o \left|\frac{p-p_o}{V_o-V}\right| = e^2$$

Let

$$V = V'/V'_o = \rho_o/\rho$$

$$(V - g)^2 V'^2_o \frac{p-p_o}{V_o (1-V)} = e^2$$

$$p - p_o = \frac{e^2 (1-V)}{V'_o (V-g)^2}$$

Now set $V'_o = 1/\rho_o$ and $\mu = \frac{1}{V} - 1$

$$(p - p_o) = \frac{e^2 \mu(1+\mu)}{[(1-g)\mu-g]^2}$$

$$p - p_o = \frac{\rho_o e^2}{g^2} \frac{\mu(1+\mu)}{\left[1-\frac{1-g}{g}\mu\right]^2}$$

$$p - p_o = \frac{\rho_o e^2}{g^2} \mu(1+\mu) \left\{ 1 + 2 \frac{1-g}{g} \mu + 6 \left(\frac{1-g}{g} \right)^2 \mu^2 + \cdots\cdots \right.$$

$$= A (1 + \mu) \left\{ 1 + 2 \frac{1-g}{g} \mu + \frac{(1-g)^2}{g^2} \mu^2 + \cdots\cdots \right.$$

$$= A [\mu + \mu^2 + 2 \left(\frac{1-g}{g}\right) (\mu^2 + \mu^3) + 6 \frac{(1-g)^2}{g^2} (\mu^3 + \mu^4) + \cdots$$